A COMPUTERIZED DATA REDUCTION SYSTEM FOR TABULATING DATA FROM GC RUNS AND CORRELATING CHANGES IN PRODUCT COMPOSITION WITH PROCESS CONDITIONS OR MUTAGENICITY

by

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Even with the sophisticated analytical instrumentation presently available, a complete and exhaustive analysis of the organics in energy or environmental samples is not only time-consuming but also difficult due to the complexity of such samples. Generally, when organic analytical analysis is done on a number of samples, a GC/MS is run on each and every sample and, for quantification, the peak area of each peak in the GC/MS total ion chromatogram or in a corresponding GC chromatogram is determined and compared to peak areas derived from standards. Since the analysis of GC/MS data is cumbersome and time consuming, typically only a few of the more important analyses are performed. If the analysis of one or more representative samples could be done by GC/MS and data of a "standard representative" sample developed, then many samples could be done "rapidly" with a GC (rather than with a GC/MS) and a data system provided the samples were similar to the "standard representative" sample.

In this study, software was developed to carry out, with the assistance of a computerized data system, the rapid analysis of a series of samples containing complex mixtures of organic compounds. One of the samples to be analyzed was chosen as a standard or reference sample. With capillary column GC/MS, it was analyzed exhaustively and identification versus retention time data were stored in the data system. To this reference sample data, identification versus retention time data from capillary column GC/MS runs on other reference samples or standard mixtures was added to make up a "super" reference sample of identification versus retention time data. Now, all samples to be analyzed were compared to this reference sample. However, in place of GC/MS, capillary column GC was used and retention time and peak area data were automatically transferred from the GC to the data system. The data system then carried out those tasks typically done by the analyst, that is, the complex sorting and matching of GC peaks, the tabulation and recording of the identification of the compounds present, the calculation and recording of the concentration, and the presentation of charts and tables for comparing the data from several samples.

The software includes programs for matching the data for several GC runs, adjusting for dilution factors and response factors, compensating for drift in retention time, multiplying in factors for presenting tables of concentration in ppb, %, µg/L, etc., and doing regression analysis on the variation in product composition as a function of such variables as process conditions or on the variation in mutagenicity as a function of product composition.

Representative output of the data system is shown in Tables 1 and 2. In Table 1, the identification, amount (in grams of compound per 100 cubic feet of LTR gas), and total for the three samples are tabulated. In Table 2, the totals for five samples (from fifteen samples) are shown. The matching of peaks, identification, determination of concentration, totaling of more than one sample, and tabulation are easily and rapidly done by the data system.

TABLE 1: SCRUB SAMPLE ANALYSIS-GRAMS OF COMPOUND PER 100 ft^3 OF LTR GAS

Compound No.	Compound Name	SAMPLE 7 Top	SAMPLE 7 Bottom	SAMPLE 8 Top	SAMPLE 8 Bottom	SAMPLE 9	Total
		.000	.000	.000	.018	.000	.018
		.000	.089	.001	.058	.010	.158
999	SOLVENT	.249	1.792	3.855	65.084	11.560	82.540
		.000	.000	.001	.000	.000	.001
		.000	.009	.002	.036	.007	.054
		.000	.000	.001	.012	.000	.013
		.000	.022	.001	.016	.005	.044
		.000	.000	.000	.007	.000	.007
1	BENZENE	2.942	.595	.380	6.445	2.530	12.891
46	THIOPHENE	.021	.003	.002	.032	.016	.073
		.007	.000	.000	.000	.000	.007
2	TOLUENE	52.181	8.030	2.261	38.748	14.523	115.743
54	METHYL THIOPHENE	.037	.000	.001	.022	.006	.066
		.000	.012	.000	.005	.000	.017
7	ETHYL BENZENE	.590	.056	.010	.173	.052	.880
6	P AND M-XYLENE	1.489	.156	.025	.441	.131	2.242
58	DIMETHYL THIOPHENE	.031	.000	.000	.000	.000	.031
59	DIMETHYL THIOPHENE	.023	.000	.000	.000	.000	.023
340	STYRENE	.042	.000	.000	.000	.000	.042
5	O-XYLENE	.390	.034	.005	.095	.027	.551
60	DIMETHYL THIOPHENE	.012	.000	.000	.000	.000	.012
25	C3-BENZENE	.359	.028	.003	.053	.012	.456
26	C3-BENZENE	.140	.010	.001	.022	.005	.179
27	C3-BENZENE	.203	.013	.001	.028	.005	.252
28	C3-BENZENE	.369	.041	.001	.026	.018	.456
29	C3-BENZENE	.122	.000	.001	.013	.000	.136
364	BENZOFURAN	.098	.000	.000	.000	.000	.098
30	C3-BENZENE	.422	.035	.003	.058	.007	.525
385	ANILINE	.150	.032	.000	.006	.000	.239
31	C3-BENZENE	.091	.000	.000	.009	.000	.101
82	INDAN	.230	.010	.001	.024	.004	.269
125	INDENE	.354	.019	.001	.029	.006	.410

Table 2: SCRUB SAMPLE ANALYSIS-TOTAL GRAMS OF COMPOUND PER 100 ft^3 OF LTR GAS (TOTALS OF THE SCRUB SETS)

Compound No.	Compound Name	SAMPLES 1-3	SAMPLES 4-6	SAMPLES 7-9	SAMPLES 10-12	SAMPLES 101-103
		.0659	.0440	.0179	.0000	.0000
		.1596	.4950	.1578	.1112	.0825
999	SOLVENT	481.5288	320.0175	82.5404	207.3195	1549.8337
		.0174	.0478	.0011	.0196	.0557
		.2053	.1447	.0543	.0930	.0364
		.0000	.0386	.0125	.0079	.0000
		.0396	.0780	.0439	.0590	.0000
		.0000	.0171	.0067	.0000	.0082
1	BENZENE	15.1490	14.3839	12.8909	17.8191	58.8526
45	THIOPHENE	.0821	.0726	.0735	.1107	.7915
		.0000	.0162	.0071	.0012	.0000
		.0000	.0310	.0000	.0454	.1285
2	TOLUENE	102.1856	138.7792	115.7428	127.2517	100.7699
54	METHYL THIOPHENE	.0369	.0646	.0659	.0900	.0000
		.0237	.0623	.0169	.0346	.0578
7	ETHYL BENZENE	.4462	.8009	.3803	.6178	.3401
6	P AND M-XYLENE	1.1335	1.9830	2.2421	1.5764	1.0254
58	DIMETHYL THIOPHENE	.0151	.0346	.0308	.0108	.0000
59	DIMETHYL THIOPHENE	.0060	.0258	.0229	.0069	.0000
340	STYRENE	.0193	.0407	.0423	.0129	.0000
5	O-XYLENE	.2553	.4709	.5512	.3523	.1730
25	C3-BENZENE	.1652	.3355	.4557	.2500	.0000
26	C3-BENZENE	.0653	.1378	.1787	.1202	.0000
27	C3-BENZENE	.0819	.1777	.2516	.0760	.0000
28	C3-BENZENE	.0965	.2803	.4560	.1119	.0000
29	C3-BENZENE	.0399	.0928	.1361	.0379	.0000
364	BENZOFURAN	.0257	.0503	.0979	.0297	.0000
30	C3-BENZENE	.1690	.3283	.5253	.2045	.0000
385	ANILINE	.0311	.1468	.2387	.0125	.1127
31	C3-BENZENE	.0295	.0665	.1007	.0233	.0000
82	INDAN	.0758	.1561	.2692	.0737	.0000
125	INDENE	.0829	.1556	.4100	.0889	.1234

Fuel

A Computerized Data Reduction System for Tabulating Data From GC Runs and Correlating Changes in Product Composition with Process Conditions or Mutagenicity

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Even with the sophisticated analytical instrumentation presently available, a complete and exhaustive analysis of the organics in energy or environmental samples is not only time-consuming but also difficult due to the complexity of such samples. More often, one is interested in such specific tasks as identifying and quantifying the major components or determining the PNAs present or determining which component or components in a fraction are causing mutagenicity.

In this study, software was developed to carry out, with a computerized data system, the rapid analysis of the major components of a complex mixture of organic compounds. With the software, one can also present data from several runs in a table in a variety of forms (%, ppb, µg/L, area counts, etc.), that is useful for making comparisons. Moreover, statistical analysis of the data can be performed such as regression analysis on the variation in product composition as a function of such variables as process conditions or on the variation in mutagenicity as a function of product composition. Such manipulations and presentations of data are rapidly handled by the data system.

A outline is presented of the software required for performing the matching of data from several GC runs, doing the adjustments for dilution factors, response factors, retention time drift, etc., multiplying in factors for presenting data in ppb, %, µg/L, etc., and doing regression analysis on the data from several runs. Data will be presented to demonstrate the performance of the data reduction system.